Quantum Computation and Quantum Spin Dynamics *

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We analyze the stability of quantum computations on physically realizable quantum computers by simulating quantum spin models representing quantum computer hardware. Examples of logically identical implementations of the controlled-NOT operation are used to demonstrate that the results of a quantum computation are unstable with respect to the physical realization of the quantum computer. We discuss the origin of these instabilities and discuss possibilities to overcome this, for practical purposes, fundamental limitation of quantum computers.

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1. Introduction

Recent theoretical work has shown that a Quantum Computer (QC) has the potential of solving certain computationally hard problems such as factoring integers [1] and searching databases much faster than a conventional computer [2]. In most theoretical work the operation of a QC is described in terms of highly idealized (but physically unrealizable) transformations on

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the qubits [3, 4, 5, 6]. The impact of the physical implementation of a QC on its computational efficiency is largely unexplored.

In this talk we discuss the relation between the physical realization of a QC and its logical operation [7, 8]. On a conventional computer or ideal QC, the order in which we execute two logically and mutually independent operations O_1 and O_2 does not matter: $O_1 O_2 = O_2 O_1$. However, a physically realizable QC is a quantum many-body system for which in general $O_1 O_2 \neq O_2 O_1$. Hence this QC may (but not necessarily does) give wrong answers. We call this problem the Quantum Programming Problem (QPP). The QPP is due to the specific physical realization of the QC and leads to systematic instead of random errors.

2. Physical Model of a Quantum Computer

We investigate the QPP by simulating QC hardware. Our choice of a physical model is largely inspired by NMR-QC experiments [9, 10, 11, 12, 13, 14, 15, 16], mainly because other candidate technologies for building QCs are not yet developed to the point that they can execute computationally non-trivial quantum algorithms (QAs). Generic QC hardware can be modeled in terms of quantum spins (qubits) that evolve in time according to the time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}|\Phi(t)\rangle = H(t)|\Phi(t)\rangle, \tag{1}$$

in units such that $\hbar = 1$. For present purposes it is sufficient to consider NMR-like two-qubit QCs only. In the absence of interactions with other degrees of freedom this spin-1/2 system can be modeled by the time-dependent Hamiltonian [17, 18]

$$
\begin{aligned}
H(t) = \; & -JS_1^z S_2^z - h_1^z S_1^z - h_2^z S_2^z - h_1^x S_1^x - h_2^x S_2^x - h_1^y S_1^y - h_2^y S_2^y \\
& -(\tilde{h}_1^x S_1^x + \tilde{h}_2^x S_2^x)\sin(\omega t + \phi_x) - (\tilde{h}_1^y S_1^y + \tilde{h}_2^y S_2^y)\sin(\omega t + \phi_y),
\end{aligned} \tag{2}
$$

where S_j^α, $\alpha = x, y, z$ denotes the α-th component of the spin-1/2 operator representing the j-th qubit, J determines the strength of the interaction between the two qubits, h_j^α and $\tilde{h}_j^\alpha$ represent the strength of the applied static (magnetic) and applied sinusoidal field (SF) acting on the j-th spin respectively. For a physical system, $h_2^\alpha = \gamma h_1^\alpha$ and $\tilde{h}_2^\alpha = \gamma\tilde{h}_1^\alpha$, for $\alpha = x, y, z$ where γ is a constant. The frequency and the phase of the SF are denoted by ω and ϕ_α. As the Ising model, i.e. the first term of (2), is known to be a universal QC [19, 20], model (2) is sufficiently general to serve as a physical model for a generic QC at zero temperature. In terms of spin matrices, the operator Q_j measuring the state of qubit j is given by $Q_j = \frac{1}{2} - S_j^z$.

For numerical purposes it is necessary to fix as many model parameters as possible. We have chosen to simulate the two nuclear spins of the ^{1}H and ^{13}C atoms in a carbon-13 labeled chloroform, a molecule that has been used in NMR-QC experiments [11, 12]. In these experiments $h_1^z/2\pi \approx 500$MHz, $h_2^z/2\pi \approx 125$MHz, and $J/2\pi \approx -215$Hz [11]. In the following we will use model parameters rescaled with respect to $h_1^z/2\pi$, i.e we put

$$J = -0.43 \times 10^{-6}, \quad h_1^z = 1, \quad h_2^z = 0.25. \tag{3}$$

With this choice of units, time divided by 2π is measured in units of 2 ns. Note that there is a difference of many orders of magnitude between the interaction J and the fields h_j^z. If the duration of the SF-pulses is much shorter than $2\pi/|J|$, the effects of J on the time evolution during these pulses are very small. Our numerical experiments (see below) are all performed under this condition. We will only consider QCs at zero temperature without coupling to the environment. In this sense we simulate highly idealized NMR experiments on a closed quantum system at zero temperature. This allows us to study a concrete physical realization of a QC and at the same time focus on its intrinsic quantum dynamics.

The time evolution of quantum model (2) is obtained by solving the TDSE (1). The simulations have been carried out with a software tool called Quantum Computer Emulator (QCE) [21]. The QCE software simulates physical models of QC hardware by a Suzuki product-formula [22, 23], i.e. in terms of elementary unitary operations [24, 25]. For all practical purposes, the numerical results obtained by this technique are exact. A detailed description of the QCE software tool can be found elsewhere [26].

3. Quantum Algorithms

One qubit is a two-state quantum system. The two basis states spanning the Hilbert space are denoted by $|\uparrow\rangle \equiv |0\rangle$ and $|\downarrow\rangle \equiv |1\rangle$. Rotations of spin j about $\pi/2$ around the x and y-axis are basic QC operations. We will denote them by X_j and Y_j respectively and write $\overline{Z}$ for the inverse of the operation Z. Clearly these operations can be implemented in terms of the time evolution of model (2) by a proper choice of the model parameters.

Computation necessarily requires some form of communication between the qubits. A basic two-qubit operation is provided by the CNOT gate. The CNOT gate flips the second spin if the first spin is in the down state, i.e. the first qubit acts as a control qubit for the second one. On an ideal QC the CNOT gate can be expressed in terms of single-qubit operations and a two-qubit phase-shift operation. There are many different, logically equivalent sequences that implement the CNOT gate on an NMR QC. Here

we limit ourselves to the sequences

$$CNOT_1 \; = \; Y_1 X_1' \overline{Y}_1 X_2' \overline{Y}_2 I' Y_2, \tag{4}$$

$$CNOT_2 \; = \; Y_1 X_1' X_2' \overline{Y}_1 \overline{Y}_2 I' Y_2, \tag{5}$$

where the symbol I' represents the time evolution $e^{i\tau(JS_1^z S_2^z + h_1^z S_1^z + h_2^z S_2^z)}$ with $\tau = -\pi/J$. The single-spin rotations X_1', Y_1', and X_2' are defined by the identities

$$e^{-i\tau(h_1^z - h)S_1^z} \; = \; Y_1 X_1' \overline{Y}_1 = \overline{X}_1 Y_1' X_1, \tag{6}$$

$$e^{-i\tau(h_2^z - h)S_2^z} \; = \; Y_2 X_2' \overline{Y}_2, \tag{7}$$

where $h = -J/2$.

As simple examples of QAs that exhibit the QPP, we consider $(QA)_1$ and $(QA)_2$ defined by

$$(QA)_1 |b_1 b_2\rangle \; \equiv \; (CNOT)^5 |b_1 b_2\rangle, \tag{8}$$

$$(QA)_2 |si\rangle \; \equiv \; Y_1 (CNOT)^5 |si\rangle, \tag{9}$$

where $|b_1 b_2\rangle \equiv |b_1\rangle |b_2\rangle$, $b_i = 0, 1$, and $|si\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$. On an ideal QC, $CNOT^2$ is the identity operation and hence $(CNOT)^5 = CNOT$. Furthermore we have $\langle si|(CNOT)^5 Q_1 (CNOT)^5 |si\rangle = 1/2$. To obtain a clear-cut, zero-one answer in terms of expectation values of the qubits we apply a $\pi/2$ rotation to spin 1: $Y_1 (CNOT)^5 |si\rangle = |11\rangle$. For this reason the CNOT operations in (9) are followed by a $\pi/2$ rotation of spin 1. Obviously, running $(QA)_1$ and $(QA)_2$ on an ideal QC yields the correct answer but as we will show below, on a physical QC this is not always the case.

It is instructive to inquire about the condition to rotate spin 1 about an angle φ_1 without affecting the state of spin 2. A general analytical, quantitative analysis of this many-body problem is rather difficult but we can easily study the limiting case in which the interaction between the spins has negligible impact on the time evolution of the spins during application of the SF pulse. This is the case that is relevant to the model system considered here (since J is very small) and also to experiments [9, 10, 11, 12]. For simplicity we consider the case of rotating SF fields, e.g. $\phi_x = 0$ and $\phi_y = \pi/2$. An SF pulse of duration t changes the state of the two-spin system according to

$$|\Phi(t)\rangle = e^{ith_1^z(S_1^z + S_2^z)} e^{it\tilde{h}_1^x S_1^y} e^{it\mathbf{S}_2 \cdot \mathbf{v}_{1,2}} |\Phi(0)\rangle, \tag{10}$$

where $\mathbf{v}_{n,m} \equiv (0, \tilde{h}_m^x, h_m^z - h_n^z)$. Without loss of generality we will assume that $0 < \gamma < 1$, in concert with the choice of parameters (3). Then, using representation (10), straightforward algebra shows that the condition to

Table 1. Model parameters of single-qubit operations on an NMR QC using rotating SFs for the case ($k = 1$, $N = 1$, $M = 4$), see (14) and (15). Parameters of model (2) that do not appear in this table are zero, except for the interaction $J = -0.43 \times 10^{-6}$, $\tilde{h}_1^y = \tilde{h}_1^x$, $\tilde{h}_2^y = \tilde{h}_2^x$, and the constant magnetic fields $h_1^z = 1$ and $h_2^z = 0.25$. The TDSE is solved using a time step $\delta/2\pi = 0.01$.

	$\tau/2\pi$	ω	$\tilde{h}_1^x$	$\tilde{h}_2^x$	ϕ_x	ϕ_y
X_1	8	1.00	-0.0312500	-0.0078125	$-\pi/2$	0
X_2	128	0.25	-0.0078125	-0.0039063	$-\pi/2$	0
Y_1	8	1.00	0.0312500	0.0156250	0	$\pi/2$
Y_2	128	0.25	0.0078125	0.0039063	0	$\pi/2$
X_1'	8	1.00	0.0559593	0.0139898	$-\pi/2$	0
X_2'	128	0.25	0.0445131	0.0111283	$-\pi/2$	0
Y_1'	8	1.00	-0.0559593	-0.0139898	0	$\pi/2$

rotate spin 1 about an angle φ_1 without affecting the state of spin 2 is given by

$$(1 - \gamma)^2 k_1^2 + \frac{\gamma^2}{4}\left(\frac{\varphi_1}{2\pi}\right)^2 = n_1^2, \tag{11}$$

where k_1 and n_1 are positive integers. Reversing the role of spin 1 and spin 2 we obtain

$$(1 - \frac{1}{\gamma})^2 k_2^2 + \frac{1}{4\gamma^2}\left(\frac{\varphi_2}{2\pi}\right)^2 = n_2^2, \tag{12}$$

where k_2 and n_2 are positive integers. The angles of rotation about the y-axis can be chosen such that $0 \le \varphi_1 \le 2\pi$ and $0 \le \varphi_2 \le 2\pi$. In general (11) or (12) have no solution but a good approximate solution may be obtained if γ is a rational number and k_1 and k_2 are large. Let $\gamma = N/M$ (for our choice of parameters, $N = 1$ and $M = 4$) where N and M are integers satisfying $0 < N < M$. It follows that the representation $k_1 = kMN^2$ and $k_2 = kNM^2$ will generate sufficiently accurate solutions of (11) and (12) if the integer k is chosen such that

$$2kNM(M - N) \gg 1. \tag{13}$$

If k satisfies condition (13) a pulse that rotates spin 1 (2) will hardly affect spin 2 (1). In terms of k, N, and M, the relevant physical quantities are then given by

$$\frac{t_1 h_1^z}{2\pi} = 2kMN^2 \quad , \quad \frac{\tilde{h}_1^x}{h_1^z} = \frac{1}{2kMN^2}\frac{\varphi_1}{2\pi}, \tag{14}$$

Table 2. Expectation values of the two qubits (a_s and b_s) as obtained on a QC that uses rotating SFs to manipulate individual qubits. The results obtained on an ideal QC are given by a and b. The time $s = \tau/2\pi = 2kMN^2$ determines the duration and strength of the SF pulses through relations (14) and (15), see Table 1 for the example of the case $s = 8$.

Operation	a	b	a_{16}	b_{16}	a_{64}	b_{64}
$(CNOT_1)^5\|00\rangle$	0.00	0.00	0.00	0.00	0.00	0.00
$(CNOT_1)^5\|10\rangle$	1.00	1.00	1.00	1.00	1.00	1.00
$(CNOT_1)^5\|01\rangle$	0.00	1.00	0.00	1.00	0.00	1.00
$(CNOT_1)^5\|11\rangle$	1.00	0.00	1.00	0.00	1.00	0.00
$Y_1(CNOT_1)^5\|si\rangle$	1.00	1.00	0.03	1.00	0.88	1.00

and

$$\frac{t_2 h_1^z}{2\pi} = 2kM^3 \quad , \quad \frac{\tilde{h}_2^x}{h_1^z} = \frac{1}{2kM^3}\frac{\varphi_2}{2\pi}. \tag{15}$$

4. Simulation of Quantum Computer hardware

The model parameters for the rotating SFs are determined according to the theory outlined above. We use the integer k to compute all free parameters and the subscript $s = 2kMN^2$ to label the results of the QC calculation. For reference we present the set of parameters corresponding to $k = 1$ in Table 1. Multiplying s (the duration of the SF pulse) with the unit of time (2 ns) shows that in our simulations, single-qubit operations are implemented by using short SF pulses that are, in NMR terminology, non-selective and hard.

In Tables 2 and 3 we present simulation results for $(QA)_1$ and $(QA)_2$ respectively. The initial states $|10\rangle$, $|01\rangle$, $|11\rangle$, and $|si\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ have been prepared by starting from the state $|00\rangle$ and performing exact rotations of the spins. It is clear that the least accurate implementation ($s = 16$) of $(QA)_1$ nicely reproduces the correct answers if the input corresponds to one of the four basis states but it is also clear that it completely fails if the input state is a singlet. In the regime where systematic phase errors are significant the QAs exhibit the QPP. This is exemplified in Table 3 where we show the results of using $CNOT_2$ instead of $CNOT_1$. For $k = 16$ there is a clear signature of the QPP: Although $(QA)_1$ and $(QA)_2$ are logically identical, the results depend sensitively on the order in which the single-qubit operations are carried out. In agreement with the theoretical analysis of Section 3 the results converge to the exact ones for sufficiently large k,

Table 3. Same as Table 2 except that instead of $CNOT_1$ sequence $CNOT_2$ given by (5) was used to perform the quantum computation.

Operation	a	b	a_{16}	b_{16}	a_{64}	b_{64}
$(CNOT_2)^5\lvert 00\rangle$	0.00	0.00	0.50	0.26	0.06	0.02
$(CNOT_2)^5\lvert 10\rangle$	1.00	1.00	0.50	0.74	0.95	0.98
$(CNOT_2)^5\lvert 01\rangle$	0.00	1.00	0.51	0.74	0.06	0.98
$(CNOT_2)^5\lvert 11\rangle$	1.00	0.00	0.50	0.26	0.95	0.02
$Y_1(CNOT_2)^5\lvert si\rangle$	1.00	1.00	0.95	0.74	0.99	0.98

as indicated in Table 2. Thus, for sufficiently slow operation this QC will operate correctly.

5. Conclusion

For each realization of QC hardware, there is a one-to-one correspondence between the QA and the unitary matrix that transforms the state of the quantum system. A QA will operate correctly under *all* circumstances if the *whole* unitary matrix representing the QA is a good approximation to the ideal one. In other words, the magnitude and the phase of *all* matrix elements should be close to their ideal values. It is not sufficient to have for example two different CNOT gates that operate correctly by themselves: Also the relative phases that they produce should match. For n qubits there are $2^n(2^n - 1)$ real numbers that specify the unitary matrix corresponding to a QA. All these numbers should be close to their ideal values, otherwise the QA is bound to produce wrong answers.

Experimental realizations of QCs have not yet demonstrated that a QC can correctly compute the answer for inputs other than simple basis states. However, with the QC hardware currently available such a test is definitly within reach. The two simple QAs, (8) and (9) may be used for this purpose.

Quantum error correction schemes that work well on an ideal QC require many extra qubits and many additional operations to detect and correct errors. The systematic errors discussed in this paper are not included in the current model of quantum error correction and fault tolerant computing [27]. On a physical QC the error-correction qubits will suffer from the same deficiencies as those discussed in this paper. All this puts considerable demands on the technology to fabricate qubits.

It remains a great challenge to demonstrate that a QC of many qubits can perform a genuine computation in less real time than a conventional computer.

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